Hydrodynamics of the zero-range process in the condensation regime

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Abstract

We argue that the coarse-grained dynamics of the zero-range process in the condensation regime can be described by an extension of the standard hydrodynamic equation obtained from Eulerian scaling even though the system is not locally stationary. Our result is supported by Monte Carlo simulations.

KEY WORDS: hydrodynamic limit; zero-range process; condensation; interacting particle systems.

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I. INTRODUCTION

The zero-range process (ZRP) was introduced in 1970 by Spitzer [1] as a system of interacting random walks, where each lattice site k is occupied by n_k particles which hop randomly to other sites. The hopping rates w_n depend only on the number of particles n at the departure site. Under certain conditions on the rates w_n and the particle density (see below) the grand-canonical stationary distribution is a product measure, i.e. there are no correlations between different sites [2]. An exact large-scale description of the *dynamics* has been proved for arbitrary initial densities in terms of a hydrodynamic equation for the coarse grained particle density $\rho(x, t')$, provided the rates are non-decreasing, i.e., $w_{n+1} \geq w_n \quad \forall \quad n$ [3, 4]. In this so-called attractive case the density satifies the continuity equation

$$\partial_{t'}\rho + \partial_x j(\rho) = 0 \tag{1}$$

where $j(\rho)$ is the stationary current in the grand-canonical distribution with density ρ.

Depending on the choice of rates, in non-attractive systems a rich and rather varied dynamical and stationary behaviour emerges, for a recent review see [5]. In particular, the model may admit a condensation phenomenon analogous to Bose-Einstein condensation. In a periodic chain one then finds that, above a critical density ρ_c, a finite fraction of all particles in the system accumulate at a randomly selected site, whereas all other sites have an average density ρ_c [6, 7, 8, 9]. The late-time dynamics of condensation has been studied in terms of a coarsening process [9, 10]. For analysis of the early time range Kaupužs et al. [11] have generalized an equivalent exclusion process for traffic flow [12]. They observed a metastable regime as a precursor of the coarsening process. The metastable state with a current above the critical current persists for some finite time range which depends on the hopping rates.

If valid, the hydrodynamic description (1) would apply to times much later than this metastable regime. Interestingly, however, the proofs for the hydrodynamic limit do not work when the condition on the rates w_n for condensation is met. The reason for this failure is *not* a minor technical issue of the standard hydrodynamic approach but lack of local stationarity during the coarsening process, the early stages of which fall within the hydrodynamic time regime. This profound violation of one of the most basic assumptions of hydrodynamic theory in conjunction with the highly discontinuous condensation phenomenon may lead one to suspect that (1) might not be valid for initial density profiles where some region of

space is above the critical density ρ_c. It is the aim of this paper to show that such a view, even though well-motivated, is overly pessimistic. We argue that, properly interpreted, the hydrodynamic limit (1) is robust and valid also in the condensation regime. The theoretical analysis of Sec. III is supported by Monte Carlo simulation in Sec. IV.

II. TOTALLY ASYMMETRIC ZERO-RANGE PROCESS

To set the stage for the new ideas in the next section, we now define the details of our model and review some known results including the hydrodynamic limit for subcritical densities.

For definiteness we consider here the one-dimensional totally asymmetric zero-range process (TAZRP) with periodic boundary conditions. The one-dimensional ZRP has attracted particular interest since it can be mapped to an exclusion processes for which double-occupancy of sites is forbidden. The ZRP-particles are turned into particle clusters between consecutive vacant sites (which correspond to the sites on which the ZRP is defined). Condensation thus corresponds to phase separation between a macroscopic particle cluster and a disordered domain which also contains vacant sites. The n-dependence of the hopping rates corresponds to a length-dependent rate of detachment of a particle from a cluster of length n. The ZRP has thus served for deriving a quantitative criterion for the existence of non-equilibrium phase separation [13] in the otherwise not yet well-understood driven diffusive systems with two conservation laws [14, 15]. Alternatively one can map ZRP-particles onto strings of vacant sites between consecutive particles (which correspond to the sites on which the ZRP is defined). In this mapping the n-dependence of the hopping rates w_n translates into a distance-dependent hopping rate for exclusion particles as may be expected for one-dimensional driven motion which is embedded in three-dimensional space. This could be of importance not only for the understanding of vehicular traffic, but also for obtaining insight into the dynamics of ribosomes along m-RNA [16] or the motion of molecular motors along microtubuli [17]. Other fields of application of the one-dimensional ZRP include experiments on condensation and metastability in granular media [18, 19].

If $\rho \leq \rho_c$ then the grand-canonical stationary product measure has one-site marginals

$P^*(n) = \text{Prob}[n_k = n]$ given by

$$P^*(n) = \frac{1}{Z}\phi^n \prod_{i=1}^{n} w_i^{-1}. \tag{2}$$

Here the empty product ($n = 0$) is defined to be 1,

$$Z = \sum_{n=0}^{\infty} \phi^n \prod_{i=1}^{n} w_i^{-1} \tag{3}$$

is the local "partition function", and ϕ is the fugacity which determines the density $\rho = \phi(d/d\phi) \ln Z(\phi)$. Due to particle conservation the product distribution defined by (2) is stationary for every ϕ for which Z exists. In the TAZRP particles hop with rate w_n from site k to site $k+1$ on a periodic chain with L sites. This process satisfies pairwise balance [20], leading to a macroscopic stationary current

$$j = \sum_{n=1}^{\infty} w_n P^*(n) = \phi. \tag{4}$$

The convexity of Z ensures that the current is an increasing function of the density. In the case of condensation the radius ϕ_c of convergence of the partition function is finite, with a critical density $\rho_c < \infty$ as ϕ approaches ϕ_c. The product measure does not exist for densities beyond ρ_c.

An intuitively convenient starting point for a coarse grained hydrodynamic description of the dynamics of the TAZRP is the lattice continuity equation

$$\frac{d}{dt}\rho_k(t) = j_{k-1}(t) - j_k(t) \tag{5}$$

for the expected local density $\rho_k(t) = \langle\, n_k(t)\, \rangle$, starting from some initial distribution. Here

$$j_k(t) = \sum_{n_k=1}^{\infty} w_{n_k} P(n_k, t) \tag{6}$$

is the expected local current with the probability $P(n_k, t) = \langle\, \delta_{n_k(t), n_k}\, \rangle$ of finding n_k particles on site k at time t. We consider Eulerian scaling where the lattice constant a (so far implicitly assumed to be unity) is taken to zero and the system is studied for rescaled time $t' = ta$, i.e., the microscopic time t is taken to infinity such that the macroscopic time t' is fixed. Since we are working with a periodic chain with L sites we take $a = 1/L$ and correspondingly $t = Lt'$. In the hydrodynamic limit $L \to \infty$ the discrete chain of L sites becomes a continuous ring of circumference 1.

We first consider the subcritical regime where initially $\rho_k < \rho_c$ everywhere on the lattice. In this case one obtains formally $\partial_{t'}\rho(x,t') + \partial_x j(x,t') = 0$ by setting $k = xL$ in the lattice continuity equation and Taylor expanding in $1/L$. In order to arrive at the continuity equation (1) one proves local stationarity which can be done rigorously for the ZRP and other lattice gas models under fairly generic circumstances. Local stationarity means that in the local environment of the point x, i.e., in a large but finite lattice region around the lattice point $x = kL$, the system is found in its stationary state. Physically, it follows from considering the limit where the microscopic time $t \to \infty$, which allows all nonconserved (fast) local degrees of freedom to relax to their local stationarity distribution at the local density ρ (which because of the conservation law is a slow dynamical variable). The identification of the expected local density $\rho(x,t')$ (appearing in (5)) with the coarse grained density of the ZRP (appearing in (1)) comes from the law of large numbers and local stationarity ensures that $j(x,t')$ is the stationary current $j(\rho(x,t'))$ computed from the product measure; for details see [4, 21].

The hydrodynamic equation (1) can be solved by writing $\partial_{t'}\rho + \partial_\rho j(\rho)\partial_x\rho = 0$ and using the method of characteristics. These are the lines $x(t') = v_{\text{char}}t'$ along which the density remains constant. The characteristic velocity is given by $v_{\text{char}}(\rho) = \partial_\rho j$. One finds smooth segments of the density which, depending on the initial data, may evolve into shocks. These are density discontinuities where the density jumps from a value $\rho_{\text{left}}(x_s,t')$ to $\rho_{\text{right}}(x_s,t')$ at the shock position x_s. Shocks travel with velocity $v_s = (j_{\text{right}} - j_{\text{left}})/(\rho_{\text{right}} - \rho_{\text{left}})$. and are stable if the Lax condition $v_{\text{char}}(\rho_{\text{left}}) > v_s > v_{\text{char}}(\rho_{\text{right}})$ is satisfied. An initial density discontinuity which does not satisfy the stability condition for shocks evolves into a rarefaction wave which is a smooth entropy solution of the continuity equation (1) [4].

On the microscopic scale, a shock is a sharp increase of the local density, averaged over a finite lattice segment. The shock position has diffusive fluctuations around its deterministic mean displacement $x_s(t') - x_s(t'_0) = v_s(t' - t'_0)$ [21]. The microscopic objects corresponding to the characteristics are spatially localized finite perturbations of the local density which travel with the collective velocity $v_{\text{coll}} = v_{\text{char}}$ of the lattice gas [22]. These microscopic perturbations are analogous to kinematic waves [23] appearing in the macroscopic PDE-description of nonequilibrium many body systems. In view of this correspondence, we shall apply the intuitively appealing term kinematic wave (in slight abuse of language) also to travelling microscopic perturbations observable on the lattice scale.

In this way one can compute the macroscopic evolution of an initial density profile provided that the initial density $\rho_0(x)$ is subcritical everywhere. For hopping rates w_n which do not lead to condensation ($\rho_c = \infty$) this is not a restriction. Furthermore, the open system behaves in a way analogous to usual lattice gases with open boundaries [24, 25, 26, 27, 28, 29]. One can compute the evolving density profile from (1) even if the condition for condensation is met, since the bulk density remains subcritical at all times [30].

III. HYDRODYNAMICS IN THE CONDENSATION REGIME

The standard considerations of the previous section fail for $\rho_0(x) \geq \rho_c$. For $\rho_0(x) > \rho_c$ the current cannot be computed from the product measure and already at $\rho_0(x) = \rho_c$ the interpretation of the characteristics as local perturbations away from the local density becomes open to doubt. A fluctuation below ρ_c would surely travel with collective velocity $v_{\text{coll}} = v_{\text{char}}$, but the interpretation of a fluctuation above ρ_c becomes dubious. In order to argue that nevertheless the continuity equation (1), properly interpreted, describes the macroscopic time evolution of the density under Eulerian scaling we now consider a supercritical density segment $\rho_0(x) > \rho_c$. The key observation is that local stationary is a sufficient, but not a necessary condition for (1) to be valid.

To fix ideas we first assume an initial distribution of particles such that the whole chain has supercritical density $\rho_k > \rho_c$. In a finite system with N particles the stationary current does not increase beyond ϕ_c in the thermodynamic limit $L, N \to \infty$ with $\rho = N/L$ fixed even though finite-size corrections can be substantial [5]. Therefore the current-density relation takes the form (Fig. 1)

$$j = \begin{cases} \phi & \text{for } 0 \leq \rho \leq \rho_c \\ \phi_c & \text{for } \rho > \rho_c. \end{cases} \tag{7}$$

This behaviour can be rationalized by viewing the site k_0 where the condensate is located in the infinite system as a source of particles which are emitted at constant rate w_∞ onto site $k_0 + 1$. On the other hand, site k_0 acts as a sink which absorbs all particles arriving from site $k_0 - 1$. The condensate site itself contains always an infinite number of particles, defined such that for every finite L one has $N = \rho L$ particles in the chain. This effectively breaks the ring into an open chain with a source at the left boundary where particles are injected with rate w_∞ and a right boundary (at $L \to \infty$) where particles are absorbed. In

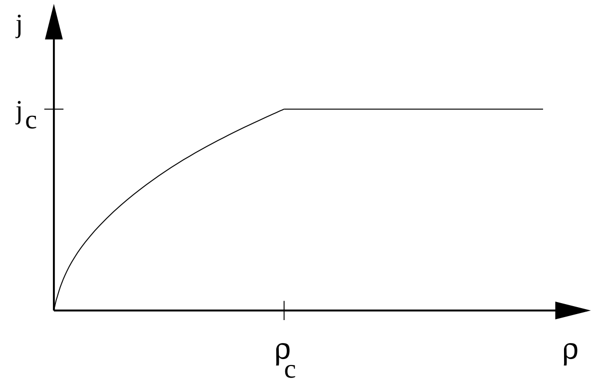


FIG. 1: Schematic picture of the stationary current density relation in the ZRP with condensation. Above the critical density the current is constant with $j_c = \phi_c$.

this case one has indeed $j = \phi_c \equiv j_c$ [24, 30].

For densities not too far above ρ_c, there is an initial metastable regime of finite duration [11]. After this the system starts to coarsen, i.e., "small" condensates at finite distance start to evolve such that larger condensates grow at the expense of smaller condensates. In the asymmetric ZRP the mean distance grows as $\sqrt{t}$ [9, 10], until eventually only a single very large condensate remains. This condensate moves on the lattice on time scales L^p where $p > 1$ depends on the details of the hopping rates [31]. We conclude that on time scales $t' = Lt$ the mean separation between condensates is proportional to $\sqrt{L}$. Hence the local density $\rho(x, t')$, coarse-grained over length segments proportional to L, remains *unchanged* on the Eulerian time scale. On the other hand, between the condensates the system has an average background density ρ_c and the current has its stationary value $j = j_c$ irrespective of ρ [9]. Therefore $\partial_x j(\rho) = 0$ and (1) is satisfied even though the system is not stationary, but coarsens.

Furthermore, one expects that kinematic waves travel with critical collective velocity $v^*_{\mathrm{coll}} \equiv v_{\mathrm{coll}}(\rho^*)$ between condensates and that they are absorbed into a condensate when they reach it after a time of order $\sqrt{L}$. Hence the long-time average collective velocity vanishes, thus allowing for identification of v_{coll} with $v_{\mathrm{char}} = \partial_\rho j = 0$ for $\rho > \rho_c$.

It remains to investigate the situation where a finite fraction of the chain is initially subcritical, whereas some neighbouring domain, also of length proportional to L, is supercritical. Inside each domain the dynamics are described by the previous considerations. In order to investigate the boundary between the domains we consider first a domain boundary

characterized by $\rho_k(0) < \rho_c$ for $k < k_0$ and $\rho_k(0) > \rho_c$ for $k \geq k_0$. We consider two piecewise constant density profiles with ρ_{left} (ρ_{right}) as the density of the subcritical (supercritical) domain. Without loss of generality we set $k_0 = 0$. Hence the two domains are connected by a density jump which on the macroscopic scale corresponds to a shock. In the supercritical domain $k > 0$ one expects at Eulerian time scale a series of small condensates, separated by a fluctuating background with average density ρ_c. We define $k_{\text{left}} = O(\sqrt{L})$ as the position of the leftmost condensate. In the whole supercritical domain the current is j_c.

In the subcritical domain ($\rho_{\text{left}} < \rho_c$) one has $j < j_c$. Hence the influx into the supercritical domain is less than the flux inside and as a result the domain boundary moves towards the first condensate. When it reaches k_{left} the flux j from the subcritical region to its left into the condensate becomes smaller than the flux j_c out of the condensate into the supercritical region. As a result the condensate shrinks in size and finally disappears. Then the domain boundary moves on until it hits the second condensate and the process of condensate annihilation sets in again. Due to mass conservation the domain boundary thus moves into the supercritical domain and "eats it up". The shock separating the two domains is stable according to the usual stability criterion since $v_{\text{left}} > v_s > v_{\text{right}}$. Notice that, as discussed above, $v_{\text{right}} = 0$ for $\rho_{\text{right}} > \rho_c$.

If $\rho_{\text{left}} = \rho_c$, mass conservation results in a vanishing shock velocity. Microscopically one expects a coarsening domain with background density ρ_c to the right of the critical domain which has $\rho = \rho_c$, but no condensates. The microscopic structure of the shock is not a jump in the background density, instead it originates from the condensates in the supercritical domain. The microscopic position of the shock is determined by the fluctuations of the position of the leftmost condensate.

Now we consider the space-reflected case where $\rho_{\text{left}} > \rho_c$ and $\rho_{\text{right}} < \rho_c$. In this case the rightmost condensate in the supercritical region serves as a source with constant flux j_c that feeds into the subcritical domain with $j < j_c$. Thus one expects a constant density profile with $\rho = \rho_c$ to the right of the rightmost condensate up to the beginning of the subcritical domain. Hence effectively one has a critical region (initially of a size of the order $\sqrt{L}$) connected to a macroscopic subcritical domain. The domain boundary moves with collective velocity v^*_{coll} and to its right a rarefaction wave develops according to the entropy solution of (1). For $v^*_{\text{coll}} = 0$ the critical domain with ρ_c does not grow on the Eulerian time scale.

Therefore, for any domain boundary between subcritical and supercritical segments, the coarse grained time evolution of the density profile can be computed from (1) with the prescription

$$v_{\text{char}} = \begin{cases} \partial_\rho j & \text{for } 0 \leq \rho \leq \rho_c \\ 0 & \text{for } \rho > \rho_c. \end{cases} \tag{8}$$

The characteristic velocity of the hydrodynamic equation and the collective velocity of the lattice gas coincide. Notice that for the TAZRP $j = \phi$ and therefore for $\rho \leq \rho_c$ the collective velocity is proportional to the inverse of the compressibility

$$\kappa = \phi \frac{\partial \rho}{\partial \phi} = \frac{1}{L}(\langle N^2 \rangle - \langle N \rangle^2) \tag{9}$$

of the lattice gas in the grand-canonical ensemble.

IV. SIMULATION RESULTS

In this section we present the results of Monte Carlo investigations which confirm the preceding theoretical analysis. We simulated a model in which particles hop to the right with rates

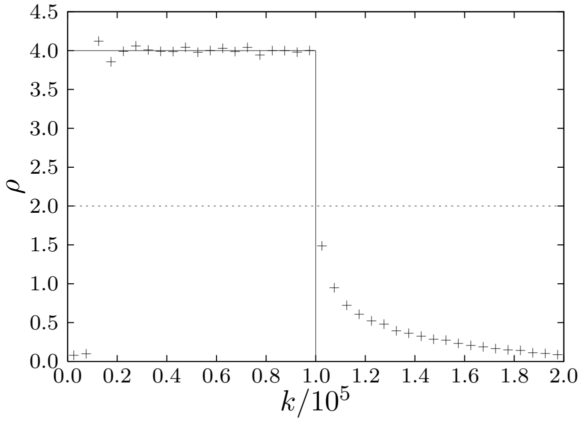
$$w_n = 1 + \frac{b}{n}. \tag{10}$$

In [6] it was observed that, for this choice of w_n, one sees condensation for $b > 2$. The critical density $\rho_c = 1/(b-2)$ and the critical collective velocity is given by [9]

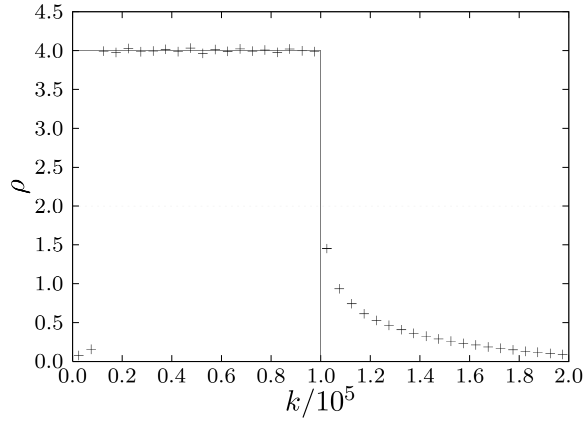
$$v^*_{\text{coll}} = \begin{cases} 0 & \text{for } 2 < b \leq 3 \\ \frac{(b-3)^2(b-2)^2}{(b-1)^2} & \text{for } b > 3. \end{cases} \tag{11}$$

Note that the collective velocity vanishes for $2 < b \leq 3$ because the compressibility is infinite.

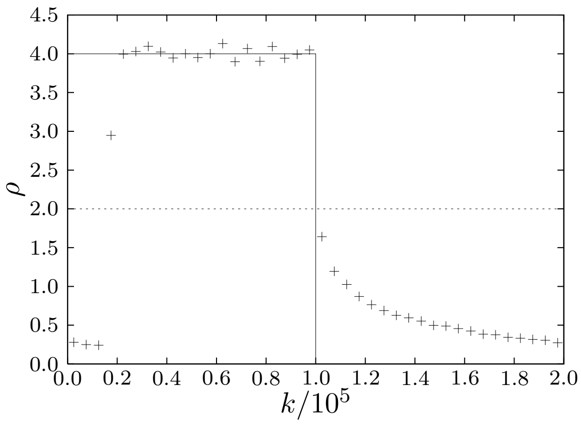
In Figs. 2 and 3 we show results for $b = 2.5$ and $b = 4$ respectively. In both cases we simulated a periodic lattice starting from an initial condition of $\rho_k(0) = 2\rho_c$ for $0 < k < L/2$ and $\rho_k(0) = 0$ elsewhere. The lefthand columns of the figures contain snapshots of the coarse-grained density profile for a single realization at increasing times whereas the righthand columns show an additional average over stochastic histories. At the left boundary of the supercritical region one clearly sees a right-moving shock front which “eats up” the condensation regime. Figure 3 also clearly demonstrates the growth of a critical domain ($\rho = \rho_c$) whose right boundary moves with a speed consistent with (11).



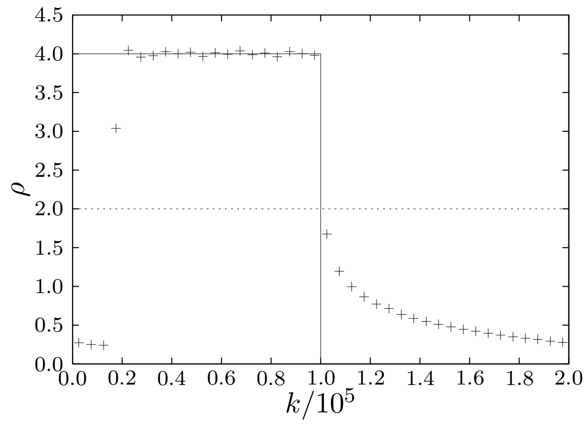
(a) $t = 0.4 \times 10^4$, single realization



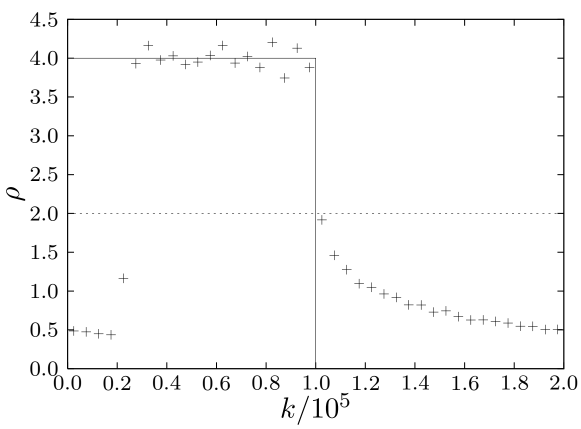
(b) $t = 0.4 \times 10^4$, average over histories



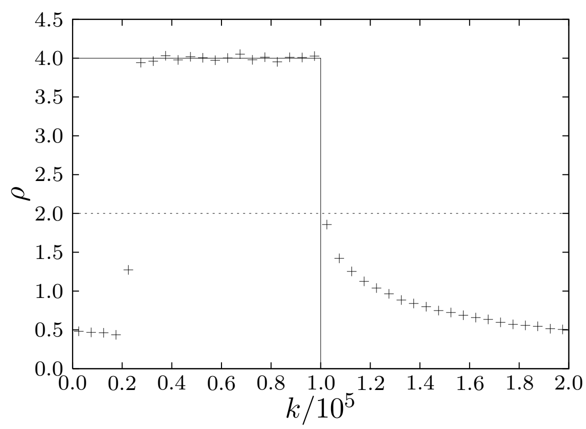
(c) $t = 0.8 \times 10^4$, single realization



(d) $t = 0.8 \times 10^4$, average over histories



(e) $t = 1.6 \times 10^4$, single realization



(f) $t = 1.6 \times 10^4$, average over histories

FIG. 2: Monte Carlo simulation results for TAZRP on a ring of size $L = 2 \times 10^5$ where w_n is given by (10) with $b = 2.5$. The data points are coarse-grained density profiles, averaged over 5×10^3 sites, at increasing times for a single realization (left column) and an average over 10 realizations (right column). The initial profile (solid line) and final density (dotted) are shown for comparison.

The ensemble average gives qualitatively the same picture as the coarse-grained space average for a single realization, thus illustrating the self-averaging nature of the process. For longer times, diffusive fluctuations smooth out the the sharp domain boundaries when the profile is averaged over histories.

V. CONCLUSIONS

In summary, we have argued that the hydrodynamic description (1) of the ZRP remains valid for supercritical densities even though locally the system is not stationary under Eulerian scaling. In order give a meaning to (1) we have analyzed the coarsening process and found that the continuity equation has to be supplemented by the results (7), (8) for the current. We have demonstrated the validity of the theory by Monte Carlo simulation of the TAZRP.

We expect similar analysis to be valid for the symmetric ZRP, under diffusive scaling $L \to \infty$ with $k = xL$, $t' = tL^2$. In this case one gets the conservation law $\partial_{t'}\rho + \partial_x^2\phi(\rho) = 0$. Inside a supercritical domain one has $\phi(\rho) = \phi_c$, corresponding to a vanishing collective diffusion coefficient. Adapting the considerations of the coarsening process to this situation one arrives at a solution that is analogous to the free boundary solution of the phase-segregation problem in the low-temperature phase of higher dimensional lattice gases [21].

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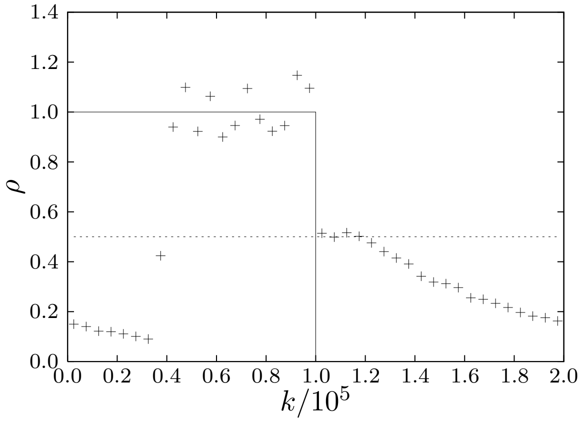
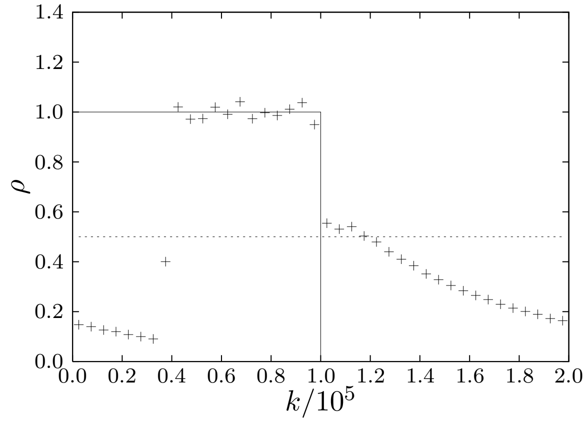
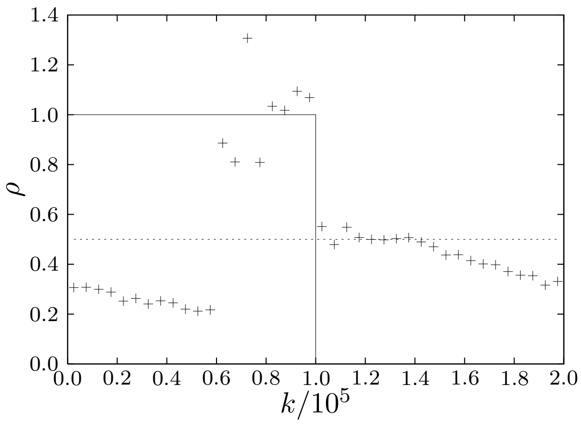


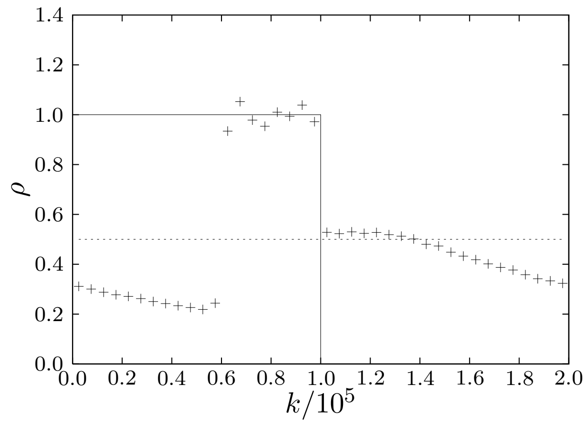
(a) $t = 0.4 \times 10^4$, single realization



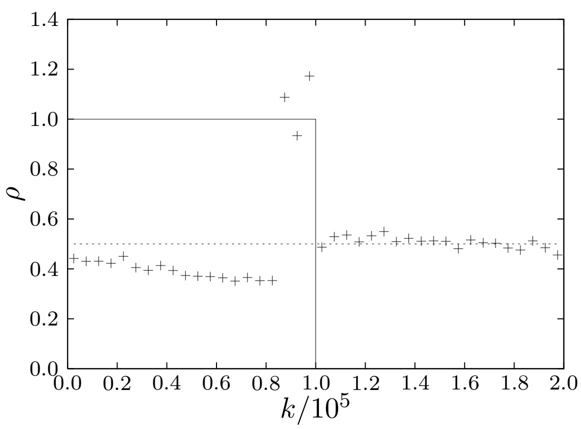
(b) $t = 0.4 \times 10^4$, average over histories



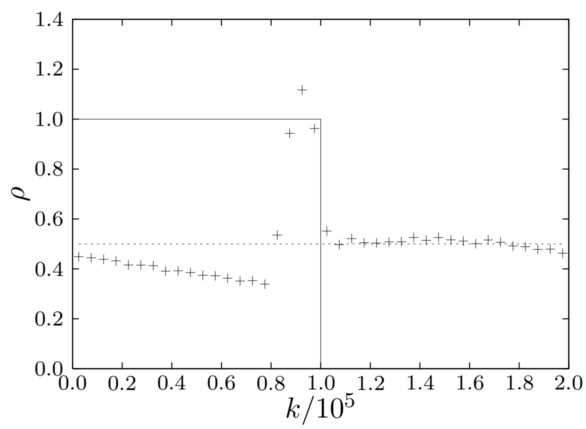
(c) $t = 0.8 \times 10^4$, single realization



(d) $t = 0.8 \times 10^4$, average over histories



(e) $t = 1.6 \times 10^4$, single realization



(f) $t = 1.6 \times 10^4$, average over histories

FIG. 3: Same as Fig. 2 but for $b = 4$. From (f) we estimate the speed of movement for the righthand boundary of the critical domain (i.e., the flat section with $\rho \approx \rho_c = 0.5$) as $7500/16000 \approx 0.47$, to be compared with the theoretical prediction, from (11), of $4/9 \approx 0.44$.